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All-Electron Ab-Initio Molecular Dynamics

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We present an all-electron implementation of the Gaussian and Augmented-Plane-Wave density functional method (GAPW method), which allows ab-initio density functional calculations for periodic and non-periodic systems. The results of the all-electron calculations for a representative set of small molecules are reported to demonstrate the accuracy and reliability of the GAPW method. Furthermore, the performance of the GAPW method is shown for some larger molecules. Finally, as a first test an all-electron ab-initio molecular dynamics (MD) run was performed for 32 water molecules in a simple cubic box under ambient conditions.